

DEPARTMENT OF PHYSICS AND ASTRONOMY  
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BOUNDARY CONDITIONS FOR THE PALEOENVIRONMENT: CHEMICAL AND  
PHYSICAL PROCESSES IN THE PRE-SOLAR NEBULA

SUMMARY OF RESEARCH (FINAL REPORT)

February 15, 1983- June 30, 1997

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Co-Principal Investigator: F. Peter Schloerb

Summary:

The basic theme of this program is the study of molecular complexity and evolution in interstellar clouds and in primitive solar system objects. Research has included the detection and study of a number of new interstellar molecules and investigation of reaction pathways for astrochemistry from a comparison of theory and observed molecular abundances. The latter includes studies of cold, dark clouds in which ion-molecule chemistry should predominate, searches for the effects of interchange of material between the gas and solid phases in interstellar clouds, unbiased spectral surveys of particular sources, and systematic investigation of the interlinked chemistry and physics of dense interstellar clouds. In addition, the study of comets has allowed a comparison between the chemistry of such minimally thermally processed objects and that of interstellar clouds, shedding light on the evolution of the biogenic elements during the process of solar system formation.

Three PhD dissertations on this research were completed by graduate students at the University of Massachusetts. An additional 6 graduate students at the University of Massachusetts and 7 graduate students from other institutions participated in research supported by this grant. Six postdoctoral research associates worked on this grant, receiving valuable training.

### Recent Research (August 1996 - June 1997):

Graduate student J. Dickens, Principal Investigator W. Irvine, and colleagues in Japan and Sweden have identified a new cyclic molecule in interstellar clouds, ethylene oxide ( $c\text{-C}_2\text{H}_4\text{O}$ ). Combining observations carried out at the NEROC Haystack Observatory in Massachusetts with data from spectral surveys made at the Nobeyama Radio Observatory in Japan and the Swedish-European Submillimeter Telescope (SEST) in Chile, they have assigned 10 observed emission lines in the Galactic center cloud Sgr B2(N) to this molecule. Ethylene oxide is a higher energy isomer of the known interstellar molecule acetaldehyde ( $\text{CH}_3\text{CHO}$ ) and of the as yet undetected species vinyl alcohol ( $\text{CH}_2\text{CHOH}$ ). Ethylene oxide is an order of magnitude less abundant than acetaldehyde in Sgr B2(N), but the combined abundances of these isomers is at least a factor of 200 larger than the predictions of recent gas phase chemical models. This suggests that the production of these relatively large organic molecules involves grain-mediated processes, consistent with previous suggestions for species such as ethanol.

The current apparitions of Comet Hale-Bopp (C/1995 O1), the intrinsically brightest comet to be observable with contemporary instrumentation, and the very close-approaching Comet Hyakutake (C/1996 B2) have provided a spectacular opportunity to study cometary chemistry and physics. We have used the University of Massachusetts' Five College Radio Astronomy Observatory (FCRAO) to make regular maps of the emission from HCN, a presumed nuclear constituent, for both comets. For the more easily observable Comet Hale-Bopp we have mapped HCN, CS (a "daughter molecule", produced by photodissociation of a parent which may be  $\text{CS}_2$ ), and  $\text{HCO}^+$ . The large extent of the emission from the latter ion, and its constantly changing morphology, manifest a previously unknown cometary phenomenon.

Observations of Comets Hyakutake and Hale-Bopp were also made in a collaborative program with astronomers from the University of Hawaii and the Joint Astronomy Centre, using the James Clerk Maxwell Telescope (JCMT) in Hawaii at submillimeter wavelengths. A principal goal of this research was to study the relationship of cometary to interstellar molecular matter, by searching for HNC, the

higher energy isomer of HCN. Under thermochemical equilibrium conditions there would be no HNC present in either environment. However, HNC is found to be relatively abundant in interstellar molecular clouds, a result that has traditionally been taken as strong supporting evidence for the validity of gas phase ion-molecule models for interstellar chemistry. Our detection of HNC in Comet Hyakutake (Irvine et al., Nature 383, 418, 1996) thus potentially provided a new chemical link between the solar system's parent molecular cloud and the solar nebula. There remains the possibility, however, that the observed cometary HNC may have been produced by photochemical processes after the comet entered the inner solar system, rather than being preserved interstellar material. In the former case the HNC/HCN abundance ratio would be expected to vary with the heliocentric distance of the comet. To investigate this phenomenon we have been making regular observations of both HNC and HCN throughout the apparition of Comet Hale-Bopp. Analysis of the data has begun.

Searches for additional molecules in the coma of Comet Hale-Bopp were made in order to study chemical composition and processes. Upper limits were obtained at various times during the apparition for  $\text{CH}_2\text{NH}$ ,  $\text{HC}_3\text{N}$ ,  $\text{CCS}$ ,  $\text{HC}_5\text{N}$  and  $\text{C}_3\text{H}_2$ , using FCRAO, the Haystack Observatory and the JCMT.

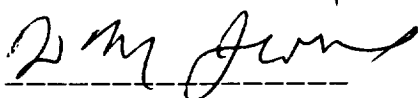
Our long-standing interest in the chemistry of regions which may become sites for solar-type star formation has stimulated the most thorough study ever attempted of the interlinked chemistry and physics of interstellar dark clouds. Two regions, Taurus Molecular Cloud One (TMC-1) and Lynds 134 North (L134N), were selected, since previous research suggested that they had similar physical properties (kinetic temperature and density) but differing compositions. Since determination of accurate molecular abundances requires knowledge of the physical conditions in the clouds, a large and diverse data set was obtained from which internally consistent values of both the physical conditions and the chemical abundances could be derived. Moreover, since the abundances are predicted to vary with the temperature and density, observations were made over extended regions of the sources to search for gradients in these physical parameters and in the corresponding chemistry. Emission from 34 rotational transitions of 22 molecular species and

isotopomers was mapped using the unique capabilities of the QUARRY focal plane array receiver on the FCRAO 14m telescope. The analysis of the results for TMC-1 is complete. Clear abundance gradients are present, which can be well matched by current models for a small variation in chemical timescales across the cloud. Such variations could easily result from slightly differing initial conditions or from a small density gradient, since the timescales depend on density.

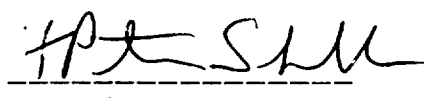
As part of their continuing study of the interplay of gas phase and grain-surface processes in interstellar clouds, Dickens and Irvine have been investigating the hydrogenation of small organic molecules. Even when such hydrogenation is energetically allowed, there are often activation barriers which are difficult to overcome at the low temperatures and densities of the interstellar medium. Following a comparison of the relative abundances of HCN and  $\text{CH}_2\text{NH}$  in both quiescent clouds and warmer regions of active star formation, they carried out a survey for  $\text{CH}_3\text{NH}_2$  in both types of region. Unfortunately, only upper limits on the abundance of  $\text{CH}_3\text{NH}_2$  were obtained for all sources outside the Galactic Center.

Irvine completed a review on the nature and distribution of extraterrestrial organic matter, based on an invited talk presented at the 1996 ISSOL meeting in Orleans, France.

Irvine attended the Symposium "The Far Infrared and Submillimetre Universe", organized by the European Space Agency in connection with planning for the FIRST mission, and presented a paper on the  $\text{HCO}^+$  observations of Comet Hale-Bopp. Schloerb presented a paper on the HCN observations of Comet Hyakutake at the 1996 meeting of the AAS Division for Planetary Sciences. Irvine was an invited participant at the NASA Ames Astrobiology Workshop in September, 1996, and helped in the preparation of the final report (NASA Conf. Publ. 10153).



W. M. Irvine, PI



F. P. Schloerb, Co-PI

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